SHORT COMMUNICATION

Pictograms for Experimental Parameters in Mass Spectrometry

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A visual documentation scheme for depicting various mass analyzers, collision-induced dissociation schemes, and mass-spectrometer and tandem mass-spectrometer scan modes are proposed. The schemes, called "pictograms," are aimed at facilitating the presentation of complex mass-spectrometry experiments on spectral outputs, figures, and schemes in research notes, presentations, and articles. (J Am Soc Mass Spectrom 1997, 8, 756–759) © 1997 American Society for Mass Spectrometry

Understanding the significance of a mass spectrum displayed in a scientific publication or presented in an oral presentation requires information about the basic experimental conditions under which the spectrum was recorded. The basic information includes specification of (i) the ionization mode, (ii) the ion polarity, (iii) the type of the mass analyzer(s), and (iv) the scan mode. This information is provided explicitly in the Experimental section and is briefly summarized in the figures. Nevertheless, when reading a publication, it is often helpful to have a comprehensive visual presentation of basic experimental parameters in addition to the corresponding mass spectrum. This should not replace a careful description in the Experimental section but should rather support a quick and unambiguous understanding of the information presented by the mass spectral data. In addition, pictograms inserted in spectra presented in oral presentations could effectively support the transfer of essential information to the audience. The benefits of pictograms are evident particularly for the documentation or presentation of data generated by tandem mass spectrometry or other complex instrumental conditions.

In the literature, there are few attempts for a visual documentation of experimental conditions under which a mass spectrum has been recorded [1, 2]. For instance, the multiplicity of fragmentation pathways in a hybrid mass spectrometer equipped with two collision cells has been visualized by a set of molecular symbols connected by arrows [1] representing the operational fundamentals of the MS/MS scan modes. This approach has been extended into a systematic outline and coining of terms for all MS/MS scan modes up to MS^3 analyses [2]. Visualization of tandem mass spectrometry conditions focused on the molecular level has the advantage of being independent of the type of mass analyzers used; however, the presentation then operates at a high level of abstraction.

In this article, pictograms are introduced that symbolize the type of mass analyzer and its mode of operation. This author feels that this approach facilitates the understanding of the important features of the analytical process, since the pictograms aim to reproduce the steps of the analytical process in a simplified manner. The operation of a mass analyzer in the scan mode is given by the corresponding symbol without any annotation; selected ion monitoring (SIM) of a single mass-to-charge ratio (m/z) value is represented by inserting the corresponding m/z value into the mass analyzer symbol, and SIM at more than one m/z value is represented by the insertion of a step symbol. This instrument-oriented approach works well for all mass spectrometry instrumentation where the functions of mass analysis and fragmentation are performed by different units within one spectrometer, e.g., a sector instrument, a hybrid instrument, a triple quadrupole analyzer, or a quadrupole/time-of-flight combination.

For an ion trap (IT) analyzer or a Fourier-transform ion cyclotron resonance (FT-ICR) cell, mass analysis and collisional activation are performed by a single unit, and thus it is difficult to create a pictogram in the same way as for the other types of instruments. Therefore, it is proposed that for IT and FT-ICR analyses, the mass analyzer pictogram be supplemented by a set of molecular symbols annotated with the corresponding m/z values. Such a display is particularly suited for the representation of multistep product ion experiments that are a special feature of IT and FT-ICR analyzers. More elaborate pictograms are not required, as by using a single unit of these mass analyzers, only product ion scans can be performed. For a description of the ionization modes, the generally accepted abbreviations have been used. The pictograms and their definitions are summarized in Figure 1.

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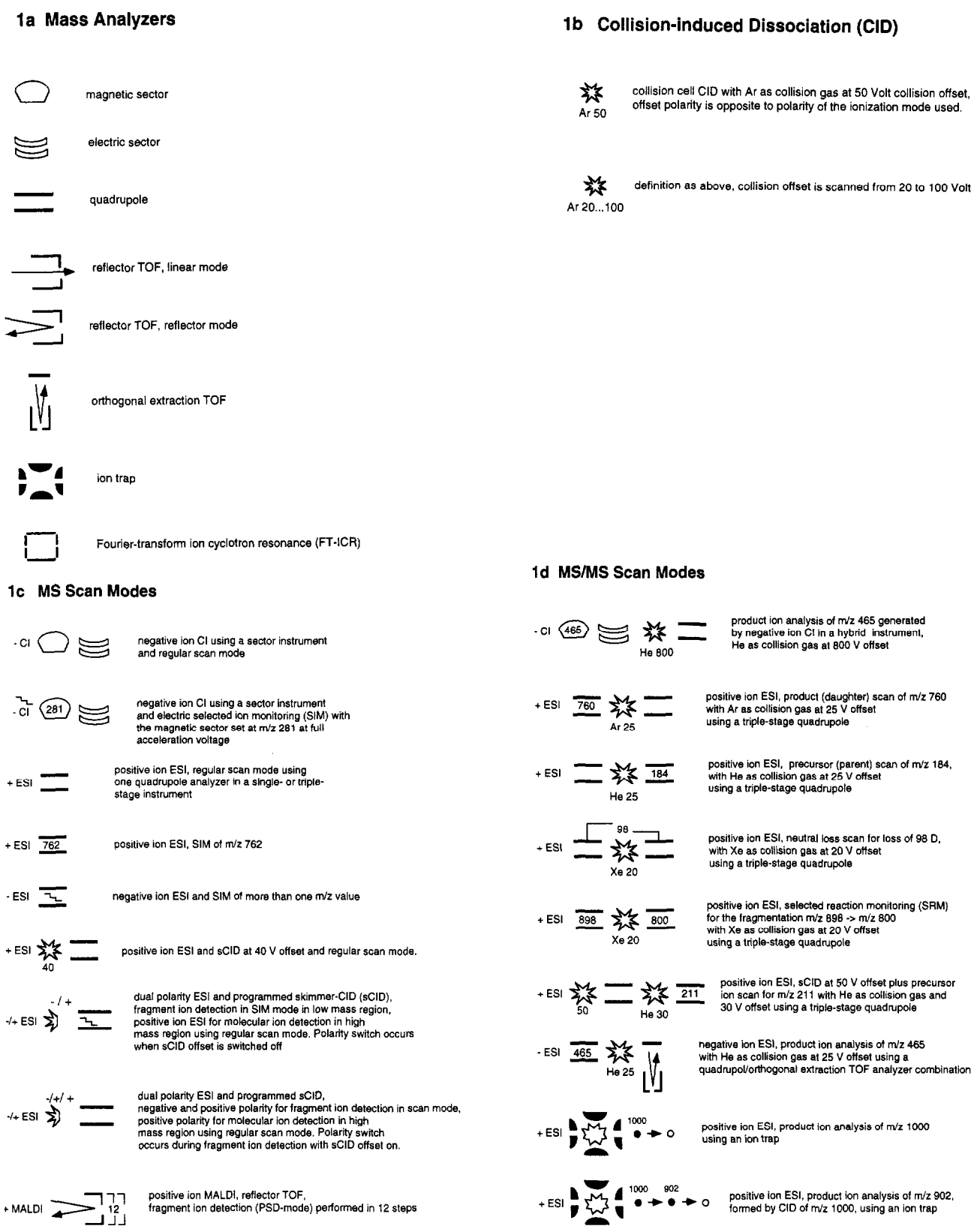

Figure 1. Definitions of pictograms for (a) mass analyzers, (b) collision-induced dissociation, (c) scan modes of mass analyzers, and (d) MS/MS scan modes.

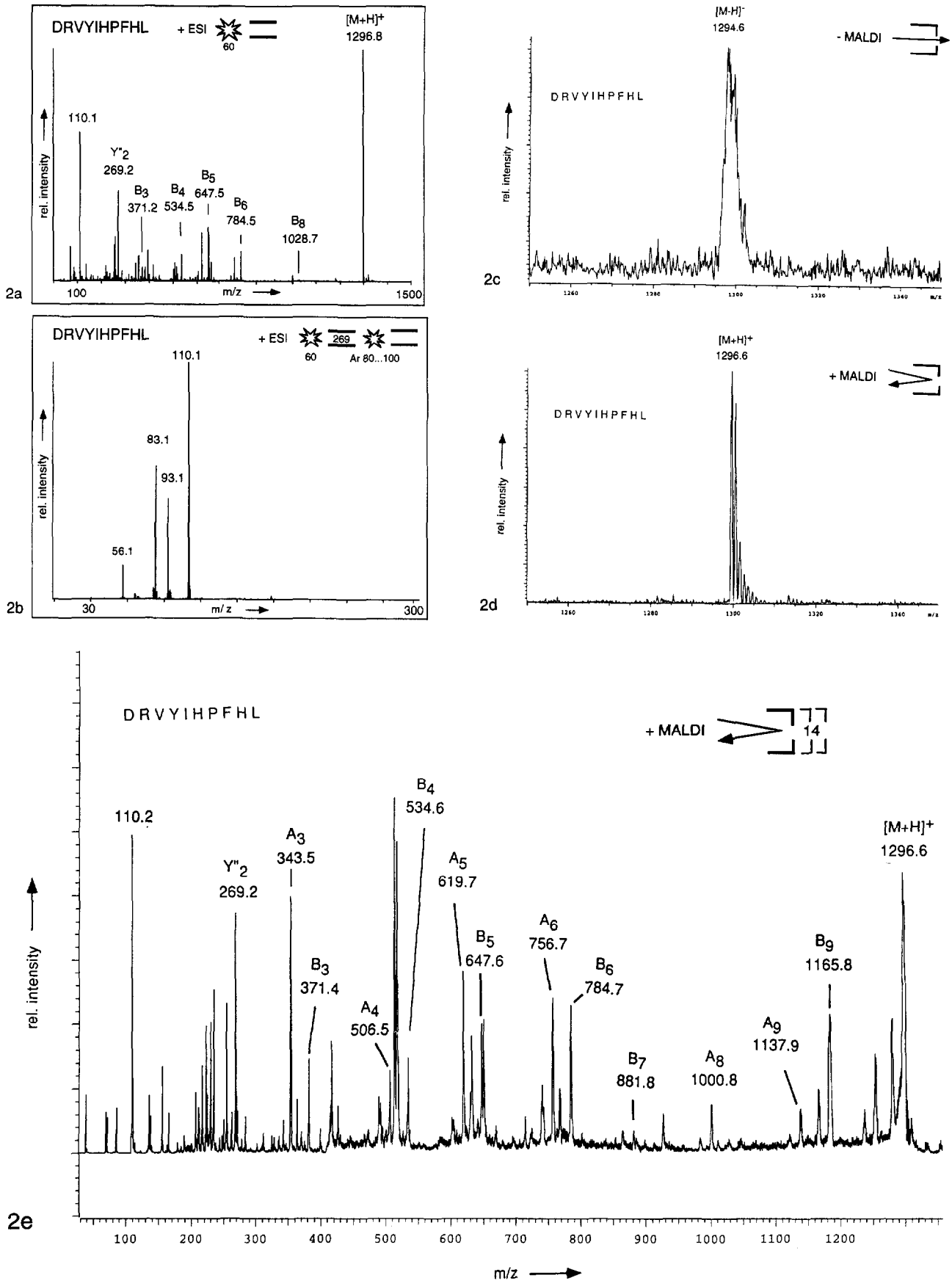

Figure 2. *(Figure continued on next page)*

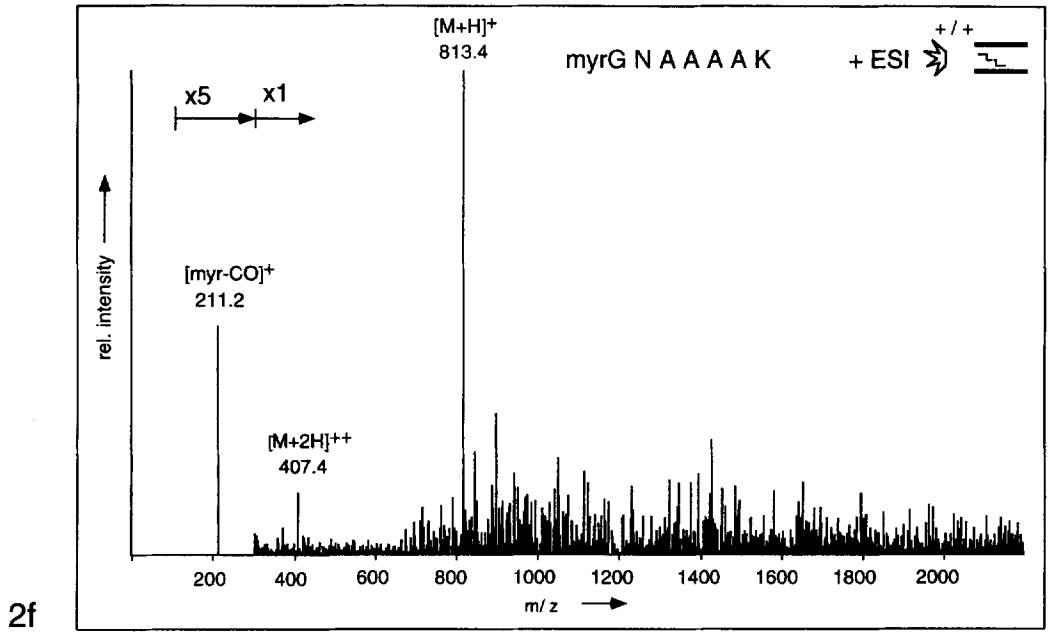

Figure 2. Mass spectra with pictogram inserts as explained in Figure 1. (a) Positive ion nanoESI mass spectrum of angiotensin I recorded with a quadrupole instrument and skimmer-CID with −60 V offset. (b) Positive ion nanoESI mass spectrum of angiotensin I recorded with a triple quadrupole instrument and two-stage collisional activation. Fragment ions were generated by skimmer-CID at −60 V offset followed by product ion analysis of the fragment at m/z 269, which was performed with a linear increase of the collision cell offset from −80 to −100 V. (c) Negative ion MALDI spectrum of angiotensin I recorded with a time-of-flight (TOF). analyzer in the linear mode and using α-cyano-4-hydroxycinnamic acid (CCA) as matrix. (d) positive ion MALDI spectrum of angiotensin I recorded with a TOF analyzer in the reflector mode and a CCA matrix. (e) Positive ion MALDI spectrum of angiotensin I recorded with a TOF analyzer in the post source decay (PSD) mode and a CCA matrix. (f) Positive ion background-subtracted ESI spectrum of the myristoylated T1 fragment of the catalytic subunit of proteinkinase A recorded with LC-ESI-MS and programmed sCID. The fragment at m/z 211 was detected in the SIM mode.

Mass spectra recorded with electrospray and matrix-assisted laser desorption using different instruments and varying scan conditions are given in Figure 2. These spectra contain pictogram inserts to demonstrate the use of the symbols shown in Figure 1. With regard to the broad and expanding variety of ionization modes, mass analyzers, and scan modes in mass spectrometry, this author feels that pictograms such as those proposed in Figure 1 represent valuable support for documentation and communication of the experimental data in this field. The concept can be expanded to visualize forthcoming innovations by creation of additional pictograms.

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